Total Records Found: 24

Start Date: Any Date

End Date: Any Date

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07/30/1999	00000056	1	104	$260.00	07/22/1999	DA 041406
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10/19/1999	00000002	1	103	-$4,248.00	07/22/1999	DA 041406
10/19/1999	00000003	1	103	-$1,962.00	07/22/1999	OP
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10/19/1999	00000006	1	201	$380.00	07/22/1999	OP
10/19/1999	**00000007**	**1**	**203**	**$763.00**	**07/22/1999**	**DA 041406**
10/19/1999	**00000008**	**1**	**203**	**$2,342.00**	**07/22/1999**	**OP**
10/19/1999	00000009	1	202	$585.00	07/22/1999	DA 041406
10/19/1999	**00000010**	**1**	**204**	**$130.00**	**07/22/1999**	**DA 041406**
10/19/1999	00000191	1	205	$65.00	10/18/1999	OP
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11/26/1999	00000004	1	203	-$763.00	07/22/1999	DA 041406
11/26/1999	00000005	1	203	-$2,342.00	07/22/1999	OP
11/26/1999	00000006	1	204	-$130.00	07/22/1999	DA 041406
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11/26/1999	00000008	4	704	-$1,946.00	07/22/1999	OP
11/20/2000	00000098	1	215	$55.00	11/16/2000	OP
11/20/2000	00000099	1	203	$72.00	11/16/2000	OP

357
+ 9

366

	L #	Hits	Search Text	DBs	Time Stamp
1	L1	796	combinatorial adj library	USPAT	2001/01/16 11:31
2	L2	14	static adj filter	USPAT	2001/01/16 11:32
3	L3	27	modelling	USPAT	2001/01/16 11:32
4	L4	0	1 and 2 and 3	USPAT	2001/01/16 11:32
5	L5	40	1 and 3	USPAT	2001/01/16 11:33
6	L6	26	5 and computer	USPAT	2001/01/16 11:33
7	L7	2	modelling and computer and combinatorial	EPO; JPO; Derwent; IBM TDB	2001/01/16 11:48
8	L8	1	modelling and combinatorial and library	EPO; JPO; Derwent; IBM TDB	2001/01/16 11:48
9	L9	1	filter and combinatorial and library	EPO; JPO; Derwent; IBM TDB	2001/01/16 11:49
10	L10	0	(static or dynamic) and combinatorial and library and model	EPO; JPO; Derwent; IBM TDB	2001/01/16 11:50
11	L11	0	(static or dynamic) and combinatorial and library	EPO; JPO; Derwent; IBM TDB	2001/01/16 11:50
12	L12	486	(static or dynamic) and modelling	EPO; JPO; Derwent; IBM TDB	2001/01/16 11:50

	L #	Hits	Search Text	DBs	Time Stamp
13	L13	3	static or dynamic and modelling and (molecule or molecules)	EPO; JPO; Derwent; IBM TDB	[illegible] 6 12:00

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FILE 'HOME' ENTERED AT 13:15:13 ON 16 JAN 2001

=> index bioscience

FILE 'DRUGMONOG' ACCESS NOT AUTHORIZED
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         1.15       1.15

INDEX 'ADISALERTS, ADISINSIGHT, AGRICOLA, ANABSTR, AQUASCI, BIOBUSINESS,
       BIOCOMMERCE, BIOSIS, BIOTECHABS, BIOTECHDS, BIOTECHNO, CABA, CANCERLIT,
       CAPLUS, CEABA-VTB, CEN, CIN, CONFSCI, CROPB, CROPU, DDFB, DDFU, DGENE,
       DRUGB, DRUGLAUNCH, DRUGMONOG2, DRUGNL, ...' ENTERED AT 13:15:24 ON 16 JAN 2001

56 FILES IN THE FILE LIST IN STNINDEX

Enter SET DETAIL ON to see search term postings or to view
search error messages that display as 0* with SET DETAIL OFF.

=> s combinatorial library and (static or dynamic) (w) filter and (model or modelling)

  16 FILES SEARCHED...
  36 FILES SEARCHED...
  45 FILES SEARCHED...

   2 FILES HAVE ONE OR MORE ANSWERS,   56 FILES SEARCHED IN STNINDEX

L1    QUE COMBINATORIAL LIBRARY AND (STATIC OR DYNAMIC) (W) FILTER AND (MODEL OR
      MODELLING)

=> s (molecule or molecular or dimensional) and (model or modelling) and library and
filter?

           9   FILE BIOSIS
           7   FILE BIOTECHNO
           1   FILE CABA
           2   FILE CANCERLIT
           3   FILE CAPLUS
  15 FILES SEARCHED...
          33   FILE CEN
           7   FILE EMBASE
           5   FILE ESBIOBASE
  33 FILES SEARCHED...
           5   FILE IFIPAT
           1   FILE LIFESCI
           7   FILE MEDLINE
          49   FILE PROMT
           9   FILE SCISEARCH
           1   FILE TOXLIT
  53 FILES SEARCHED...
         [illegible]   FILE USPATFULL
           2   FILE WPIDS
           2   FILE WPINDEX

  17 FILES HAVE ONE OR MORE ANSWERS,   56 FILES SEARCHED IN STNINDEX

L2    QUE (MOLECULE OR MOLECULAR OR DIMENSIONAL) AND (MODEL OR MODELLING) AND LI
      BRARY AND FILTER?

=> d rank
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F1 - -      6305   USPATFULL
F2            49   PROMT
F3             3   CEN
F4             4   BIOSIS
F5             4   SCISEARCH
F6             7   BIOTECHNO
F7             7   EMBASE
F8             7   MEDLINE
F9             5   ESBIOBASE
F10            9   IFIPAT
F11            3   CAPLUS
F12            2   CANCERLIT
F13            2   WPIDS
F14            2   WPINDEX
F15            1   CABA
F16            1   LIFESCI
F17            1   TOXLIT


=> file f3-f17

COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
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FILE 'TOXLIT' ENTERED AT 13:19:23 ON 16 JAN [illegible]

=> s l2; dup rem l3

    5 FILES SEARCHED...
   12 FILES SEARCHED...
L3   99 L2

PROCESSING COMPLETED FOR L3
L4   59 DUP REM L3 31 DUPLICATES REMOVED.

=> d 1-59 bib ab; log h

:MALII *TIB-ACC-NO: NN8702771

DISCLOSURE TITLE: Software Package for Molecular Modelling and Structural Characterica- Tion

PUBLICATION-DATA: IBM Technical Disclosure Bulletin, February 1987, US

VOLUME NUMBER: 29

ISSUE NUMBER: 9

PAGE NUMBER: 3771 - 3773

PUBLICATION-DATE: February 1, 1987 (19870201)

CROSS REFERENCE: 0018-8689-29-9-3771

DISCLOSURE TEXT:

- The difficulty in comparing complicated molecular structures and phenomena motivates the development of these software packages, systems, and methods. The highly interactive nature of their user interfaces and the variety of data representations available to the user suggest the extension of these analyses beyond the biomolecular domain. A set of software is disclosed which facilitates the structural and dynamical characterization of biomolecules (or other large molecules). The various routines currently run on an IBM 3277 GA and Tektronix Graphics display. The support software is PL/I, and the interactive graphics language is GCS. The Random-Dot Display

Program makes use of a moire interference pattern to allow researchers to compare orientations of structural parts, such as protein subunits.

Method: If a pattern of random dots is superimposed on itself and rotated by a small angle, concentric circles are perceived about the point of rotation. If the angle of rotation is increased, the perceived circles gradually disappear until a totally unstructured dot display is seen. This effect demonstrates the ability of the human visual system to detect local autocorrelations and may suggest a physiological basis of form perception in higher animals. Demonstration: This graphical technique may be used in situations where two conformers of a lobed molecule are known and an equivalent axis of rotation relating the two is desired. First, two identical random-dot patterns are superimposed over the computer graphics representation of one form of the protein. One of the dot patterns is rotated along with one lobe until the lobe is in its new position, while the other remains with the stationary lobe. Even a small change, represented by a one-degree rotation of one lobe relative to the other, creates a figure where the axis of rotation can begin to be perceived at the center of the concentric circles.

DNA Spectrogram and Power Spectra - Two useful ways of describing base content and periodicity for nucleic acid sequences are the

spectrogram and three-dimensional power spectrum, representations similar to those frequently used in the field of digital signal processing. The user assigns a numerical value to each of the DNA bases (G,C,A,T), thereby converting the string of characters to a digitized waveform.

The user also specifies a data window (i.e., how many contiguous bases will be characterized in each strip of the output display) and a window overlap (how many bases the adjacent windows have in common). If the user desires to focus on smaller regions of the DNA and is not concerned with low frequency patterns, a small window may be chosen. If the user desires a more global characterization of the patterns within the DNA sequence, a large window is chosen. The overlap parameter makes it easier to capture the spatial dynamics of the features of interest. In both the 3-D power spectrum and spectrogram, the mean window value is subtracted, and Hamming cosine tapers are first applied to each window of data prior to fast Fourier transformation.

Hillocks in the three-dimensional spectrum, and darkness on spectrogram, indicate prominent periodicities in the input sequence; the more common the periodicity, the greater the intensity. Since both the spectrogram and 3-D power spectrum present nucleic acid sequence data in a way which can be visually interpreted by the molecular geneticist, a variety of nucleotide sequence characterizations is

facilitated. This technique has been successfully applied to detect the spatial evolution of sequence periodicities in a human bladder cancer gene analysis.

Spectrographic representation of protein breathing motions - A complete description of a globular protein requires not only a static three-dimensional x-ray structure, but also an understanding of its flexibility and the role that structural fluctuations play in the protein's function.

Globular proteins in solution exhibit a large variety of motion. As above, 3-D power spectra can be applied to the study of such molecular motions. In particular, "low frequency" vibrations of globular proteins, corresponding to the collective oscillations of atoms from many different residues, can be considered. Radii of gyration fluctuations provide a sensitive way to characterize such concerted motions. In the current work, a research system for the computation of digital spectrograms and topographic spectral distribution functions of protein breathing motions was developed.

For the tipographic power spectrum (amplitude vs. frequency vs. time), hillocks are indicative of prominent periodicities in the concerted radial motions within the protein.

When applied to a small protein (bovine pancreatic trypsin inhibitor) a 3-D power spectrum computed for the Rg fluctuations indicates most of the frequency power below 1 ps with a particularly prominent

breathing mode centered at 3 ps. Since both the spectrogram and 3-D power spectrum present breathing motion data in a way which can be easily understood by the biophysicist, characterization of the dynamical richness of proteins is greatly facilitated. DNA Face Icon - This visual method of data reduction is accomplished by computer-drawn faces which function as multivariate representations sensitive to regularities and irregularities of the statistical properties of the sequence of bases.

Various graphical methods of representing multivariate data using icons, or symbols, have been discussed previously. The system presented here is special in that it has as its primary focus the rapid characterization of a multi-dimensional data series using an interactive graphics system with a variety of controlling parameters. In general, n data parameters are each mapped into a figure with n features, each feature varying in size or shape according to the point's coordinate in that dimension. One particularly novel method of representing multivariate data has been presented by Chernoff.

The data sample variables are mapped to facial characteristics; thus, each multivariate observation is visualized as a computer drawn face. Such faces have been shown to be more reliable and more memorable than other tested icons and allow the human analyst to grasp many of the essential regularities and irregularities in

the data. In this disclosure, faces are used to represent statistical properties of the sequence of bases in the DNA of a human bladder cancer gene. In order to use the system for a DNA sequence, a file containing a listing of the nucleic acid bases (G, C, A, T) is required. The user specifies a window size (how many contiguous bases will be represented in each face of the output display, e. g., 100 bases), and the program then automatically marches through the sequence, drawing one face for each window.

In the current applications, ten facial parameters, F(1,2,3,4, 5,6,7,8,9,10), are used, and each facial characteristic has ten settings, S(1,2,3,4,5,6,7,8,9,10). The simplest way to take specific sequence interactions into account is to assume that all effects are dominated by nearest-neighbor interactions. In this disclosure, the occurrences of the 10 possible neighbor pairs (GC,GA,GT,GG,CA,CT,CC, TA,TT,AA) are individually summed within a data window, and the deviation of the sums from the expected (random) value causes deviations of the facial parameters from their middle positions. The computer-drawn faces were calculated and displayed for a human bladder oncogene. The computer-drawn faces allow one to detect substantial changes in the base composition along a gene sequence. A massive amount of data is condensed into a small number of faces.

In summary, the icons presented in this disclosure provide a qualitative awareness of complex DNA sequence trends, and may subsequently guide the researcher in applying more traditional statistical calculations. They point out regularities and irregularities in the DNA sequence which are not easy to observe using conventional techniques. Overall Feature Summary - Graphics are generally limited to a finite number of dimensions, requiring that many multivariate data problems be reduced to fewer dimensions before analysis. The various techniques and programs described here are useful in allowing a user to detect and comprehend important phenomena and for communicating major conclusions to others.

What makes the graphics system described here special is its primary focus on the rapid characterization of a dynamic sequence of data using an interactive graphics system with a variety of controlling parameters.